Specific heat and energy for the three-dimensional $O(2)$ model *

S. Holtmann with J. Engels and T. Schulze

Fakultät für Physik, Universität Bielefeld,
D-33615 Bielefeld, Germany

We investigate the three-dimensional $O(2)$ model on lattices of size 8^3 to 160^3 close to the critical point at zero magnetic field. We confirm explicitly the value of the critical coupling J_c found by Ballesteros et al. and estimate there the universal values of g_r and ξ/L. At the critical point we study the finite size dependencies of the energy density ϵ and the specific heat C. We find that the nonsingular part of the specific heat C_{ns} is linearly dependent on $1/\alpha$. From the critical behaviour of the specific heat for $T \neq T_c$ on the largest lattices we determine the universal amplitude ratio A^+/A^-. The α-dependence of this ratio is close to the phenomenological relation $A^+/A^- = 1 - 4\alpha$.

1. INTRODUCTION

$O(N)$ models in three dimensions play an important part in condensed matter physics and in quantum field theory, because many systems belong to the corresponding universality classes. In three dimensions the case $N = 2$ is a special one, because the $O(2)$ model is the first $O(N)$ model (with increasing N) exhibiting massless Goldstone modes. Furthermore its critical exponent α, which controls the critical behaviour of the specific heat, is negative and very close to zero. In the famous shuttle experiment [1] the universal ratio A^+/A^- and α have been determined experimentally. Here we want to calculate this ratio from Monte Carlo simulations.

The $O(2)$-invariant nonlinear σ-model (or XY model) for zero magnetic field, which we examine here, is defined by the partition function

$$Z \;=\; \int [d\vec{\phi}] \exp[J \sum_{<i,j>} \vec{\phi}_i \cdot \vec{\phi}_j]. \tag{1}$$

Here $\vec{\phi}_x$ is a 2-component unit vector at site x and $J = 1/T$ is the inverse temperature. We use the lattice average of the spins

$$\vec{m} \;=\; \frac{1}{V}\sum_i \vec{\phi}_i \quad \text{with} \quad V = L^3 \tag{2}$$

to define the magnetization M, the order parameter of the system, by

$$M \;=\; \langle |\vec{m}| \rangle , \tag{3}$$

the susceptibility χ

$$\chi \;=\; V \left\langle \vec{m}^2 \right\rangle , \tag{4}$$

and the Binder cumulant g_r

$$g_r \;=\; \frac{\left\langle (\vec{m}^2)^2 \right\rangle}{\left\langle \vec{m}^2 \right\rangle^2} - 3. \tag{5}$$

The second moment correlation length ξ_{2nd} is calculated from

$$\xi_{2nd} \;=\; \left(\frac{\chi/F - 1}{4\sin^2(\pi/L)} \right)^{1/2}, \tag{6}$$

where F is the Fourier transform of the correlation function at momentum $p_\mu = 2\pi\hat{e}_\mu/L$. Important observables for this work are the energy E, the energy density ϵ

$$E \;=\; -\sum_{<i,j>} \vec{\phi}_i \cdot \vec{\phi}_j \quad , \quad \epsilon \;=\; \frac{\langle E \rangle}{V} \tag{7}$$

and the specific heat C

$$C \;=\; \frac{\partial \epsilon}{\partial T} \;=\; \frac{J^2}{V}(\left\langle E^2 \right\rangle - \langle E \rangle^2). \tag{8}$$

*Talk given by S. Holtmann, this work was supported by DFG Grant No. FOR 339/1-2.

At the critical coupling J_c the finite size behaviour of the energy density is

$$\epsilon(L) \;=\; \epsilon_{ns} + q_\epsilon\, L^{\frac{\alpha-1}{\nu}}\,, \tag{9}$$

and that of the specific heat

$$C(L) \;=\; C_{ns} + q_c\, L^{\frac{\alpha}{\nu}}\,(1 + q_{1c} L^{-\omega}). \tag{10}$$

ϵ_{ns} and C_{ns} are the nonsingular parts of the energy density and of the specific heat, respectively. In the thermodynamic limit the critical behaviour of C for T close to T_c is

$$C(t) \;=\; C_{ns} + \frac{A^{\pm}}{\alpha}\,|t|^{-\alpha}\,[1 + c_1^{\pm}\,|t|^{\omega\nu} + c_2^{\pm}\,t], \tag{11}$$

where $t = (T - T_c)/T_c$ is the reduced temperature. Here correction to scaling terms have been included. We use the first irrelevant exponent $\omega = 0.79(2)$ from [2] in the following fits.

2. NUMERICAL RESULTS

Our simulations were done on three-dimensional lattices with periodic boundary conditions and linear extensions $L = 8 - 160$ using the Wolff single-cluster algorithm.

First we have determined again the critical coupling J_c, utilizing the fact that Binder's cumulant should be finite size independent at criticality. We have interpolated data from simulations on lattices with $L = 24, 36, 48, 72$ and 96. The curves for the different lattices do not cross in a single point due to small corrections to scaling. Including these we find that the shift Δ from criticality of the crossing point between two lattices of size L and L' $(b = L'/L)$ is

$$\Delta J_c^{L,L'} \;\propto\; \frac{1 - b^{-\omega}}{b^{1/\nu} - 1} L^{-\omega - 1/\nu}. \tag{12}$$

The ν-dependence of $\Delta J_c^{L,L'}$ is not relevant as long as $\nu \in [0.669; 0.675]$. Extrapolating to $L \to \infty$ we find the value

$$J_c = 0.454167(4), \tag{13}$$

in agreement with $J_c = 0.454165(4)$ from [3]. In a similar way we determine the universal values of g_r and ξ_{2nd}/L at J_c to

$$g_r = -1.758(2) \quad \text{and} \quad \xi_{2nd}/L = 0.593(2), \tag{14}$$

in accordance with [4] and [2].

In order to estimate the nonsingular parts ϵ_{ns} and C_{ns} of the energy density and the specific heat the finite size effects of these observables at T_c were studied. The model was simulated at $J_c = 0.454165$ on lattices with $L = 8$ to $L = 160$. Fits to the data with Eqs. (9) and (10) show no corrections to scaling in case of the energy density and only small corrections for the specific heat. The quantity ϵ_{ns} exhibits no noticeable dependency on ν, and we find $\epsilon_{ns} = -0.98841(3)$. When we treat ν as a free fit parameter, we get 0.671(2). In case of the specific heat the situation is different. Its nonsingular part varies from about 50 for $\nu = 0.669$ to 16 at $\nu = 0.675$. This is so because the exponent α/ν in Eq. (10) is approximately zero. As shown in Fig. 2 the nonsingular part of the specific heat C_{ns} is linearly dependent on $1/\alpha$. We find

$$C_{ns}(\alpha) \;=\; 3.35(26) \;-\; \frac{0.3176(43)}{\alpha}. \tag{15}$$

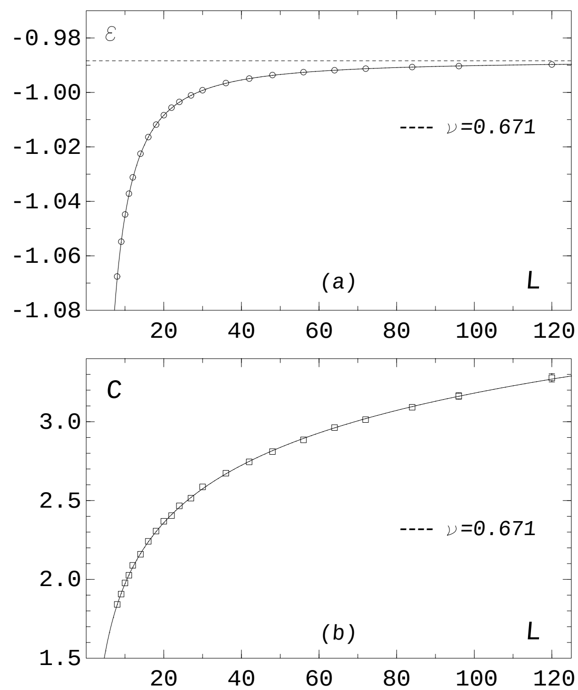

Figure 1. The energy density (a) and the specific heat (b) vs. L at criticality. The dashed line shows ϵ_{ns} and the solid lines fits for $\nu = 0.671$.

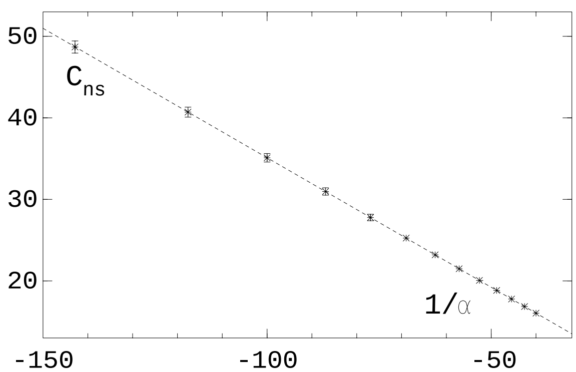

Figure 2. The nonsingular part of the specific heat. The dashed line is the fit (15).

This result for C_{ns} is used to analyse the specific heat at $T \neq T_c$ and $V \to \infty$. Our data are shown in Fig. 3. We have interpolated the data from the largest lattices by reweighting. The resulting curves have been fitted to the form (11). In the broken phase the correction to scaling terms in the bracket are relevant for the fit, whereas these terms are negligible for $T > T_c$. Again we observe an α-dependency in the fit parameters, especially for the amplitudes $A^{\pm}$:

$$
\begin{aligned}
A^{+} &= 0.3177(2) - 3.29(4)\alpha + 18.8(1.3)\alpha^2 \quad (16)\\
A^{-} &= 0.3176(3) - 1.97(4)\alpha + 7.8(1.4)\alpha^2. \quad (17)
\end{aligned}
$$

As expected, we obtain the same amplitudes for $\alpha \to 0$, and the $1/\alpha$-pole term in C_{ns} is cancelled exactly there: the same specific heat data can as well be fitted at $\alpha = 0$.

The universal ratio A^+/A^- can now be written as

$$A^+/A^- \;=\; 1 - 4.23(3)\alpha + 3.3(1.8)\alpha^2 + \ldots\,. \quad (18)$$

It is shown as solid line in Fig. 4. This result is well in accordance with former results, e.g. from the shuttle experiment [1] and analytic determinations [4] and [5]. The leading part is also close to the phenomenological relation [6]

$$A^+/A^- = 1 - 4\alpha\ . \quad (19)$$

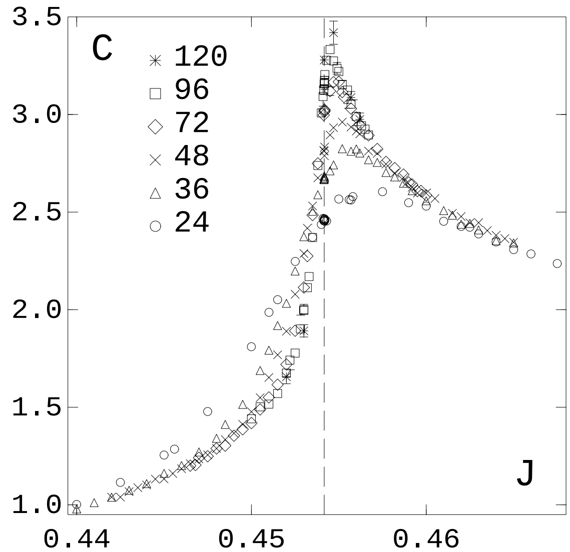

Figure 3. The specific heat for different L vs. the coupling J. The line shows the position of J_c.

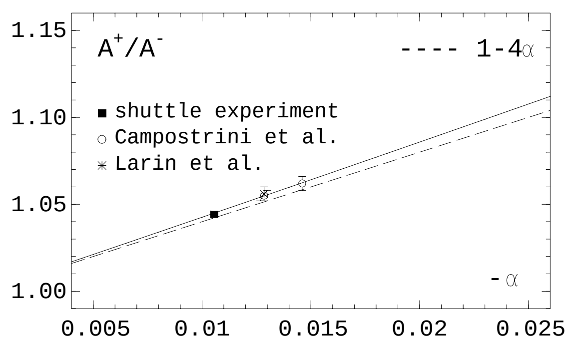

Figure 4. The universal ratio A^+/A^- as a function of $-\alpha$. The solid line shows the result (18).

REFERENCES

1. J.A. Lipa et al. , Phys. Lett. **84** (2000) 4894.
2. M. Hasenbusch and T. Török J. Phys. A**32** (1999) 6361.
3. H.G. Ballesteros et al. , Phys. Lett. B**387** (1996) 125.
4. M. Campostrini et al. , Phys. Rev. B**63** (2001) 214503.
5. S.A. Larin et al. , Phys. Rev. B**58** (1998) 3394.
6. P.C. Hohenberg et al. , Phys. Rev. B**13** (1976) 2986.